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1. **The Ising model**. The Ising model is named after Ernst Ising, Ph.D. in Physics (1924) from the University of Hamburg under the supervision of Wilhelm Lenz. Ising solved the one-dimensional (1D) Ising model exactly to find no phase transition. He also provided arguments on why there would not be a phase transition in higher dimensions either. In 1936, Peierls argued that both 2D and 3D Ising models admit phase transitions. Read the paper of Peierls [1] and explain the arguments.

   The Ising Hamiltonian can be written as,

   $$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j.$$

   (a) The spins σ_i can take values ± 1 on the ith lattice site.

   (b) $\langle ij \rangle$ implies nearest-neighbor interaction only,

   (c) $J > 0$ is the strength of exchange interaction.

   The system undergoes a second order phase transition at the critical temperature T_c in two and higher dimension. For temperatures less than T_c, the system magnetizes in an ordered state. For temperatures greater than T_c, the system is in the disordered state. In this case, there are no long-range correlations between the spins. The order parameter

   $$m = \frac{1}{N} \sum_i \sigma_i$$

   for this system is the average magnetization. The order parameter distinguishes the two phases realized by the systems. It is zero in the disordered state, while non-zero in the ordered state.

   (a) The Ising Model has no explicit dynamics. Simulate (or download a code from the internet [2]) Ising model using the Metropolis algorithm, whose steps are:

      i. Prepare an initial configuration of N spins

      ii. Flip the spin of a randomly chosen lattice site.

iii. Calculate the change in energy dU.

iv. If $dU < 0$, accept the move. Otherwise accept the move with probability $e^{-\beta dU}$. Here $\beta = 1/(k_B T)$

v. Repeat (ii)-(iv).

(b) Check that the Metropolis algorithm satisfies the condition of detailed balance.

(c) Plot the following quantities as a function of T from your simulation in one and two-dimensions.

- Order parameter (magnetisation): m
- Energy $U = \langle E \rangle$
- Specific heat $C = \dfrac{\partial U}{\partial T} = \dfrac{\langle E^2 \rangle - \langle E \rangle}{k_B T^2}$
- Susceptibility: $\chi = \dfrac{\partial m}{\partial h} = \dfrac{\langle M^2 \rangle - \langle M \rangle}{k_B T}$

(d) Solve the Ising model exactly in one-dimenion using the transfer matrix method.

2. Solve problem 1 of chapter 1 of Kardar's book (Statistical Physics of Fields).

3. Solve problem 2 of chapter 1 of Kardar's book (Statistical Physics of Fields).

4. **Legendre transformation and thermodynamic potentials.**

(a) Explain the concept of Legendre transformations.

(b) Explain the concept of thermodynamic potentials.

(c) What are extensive and intensive variables in thermodynamics?

(d) The change in internal energy U of a system is:

$$dU = TdS - PdV + \mu dN \tag{1}$$

Here μ is the chemical potential. The internal energy U can be considered as a function of S, V and μ. In some situations of experimental interest, it may be useful to have other independent variables. Find the independent variables for the following thermodynamics potentials:

- Helmholtz Free energy: $F = U - TS$
- Gibbs Free energy: $G = F + PV = U - TS + PV$

- Enthalpy: $H = U + PV$

(e) Show that: $G = \mu N$.

(f) The variations of intensive coordinates variables is constrained:

$$SdT - VdP + Nd\mu = 0 \tag{2}$$

The above is called the Gibbs-Duhem relation. Prove the relation and explain its significance.

5. **van der Waals equation of state.** The van der Waals equation is given as

$$\left(P + \frac{a}{v^2}\right)(v - b) = k_B T.$$

Here v is the volume per unit particle. The van der Waals equation of state reduces to the idea gas equation $Pv = k_B T$ when the constants a and b are zero.

(a) Explain the origin of the constants a and b?

(b) Determine change in pressure with volume at constant temperature $(\partial P/\partial v)_T$

(c) Find the critical temperature T_c below which the mechanical stability is lost.

(d) Sketch P as a function of V for temperatures above and below T_c.

6. **The exact equivalence between the Lattice Gas Model and Ising Model**. In the lattice gas model, each site maybe occupied by a fluid molecule. The fluid molecules interact via the potential $V(r)$, which is given as:

$$V(r) = \begin{cases} \infty & (r = 0) \\ -U & (r = a) \\ 0 & \text{otherwise} \end{cases}$$

Thus, two fluid particle on nearby site reduce energy by U. Otherwise there is no interaction if nearby site is empty. The Hamiltonian for the Lattice Gas Model is written as:

$$H = -\sum_{<ij>}^{N} U\, c_i\, c_j - \mu \sum_{i=1}^{N} c_i \tag{3}$$

(a) Show that the above model in Eq.(3) is exactly equivalent to the Ising model:

$$H = -\sum_{\langle ij \rangle}^{N} J\,\sigma_i\,\sigma_j - h\sum_i \sigma_i \tag{4}$$

Here $J > 0$ and $\sigma = \pm 1$.

(b) The transformation can be achieved by the transformation: You may use the transformation $\sigma_i = f(c_i)$. Find the exact form of $f(c_i)$.

(c) Show that the transformation results in the following:

$$J = \frac{U}{4}, \qquad 2h = zU + \mu. \tag{5}$$

[1] Peierls, Rudolf. On Ising's model of ferromagnetism. 1936.

[2] See for example: https://rajeshrinet.github.io/blog/2014/ising-model/.